

Supporting Information

Luminescent Hybrid Halides with Various Centering Metal Cations (Zn, Cd and Pb) and Diverse Structures

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{Bmpip})_2\text{ZnBr}_4$ at 293(2) K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Br(1)	6169(1)	9624(1)	1527(1)	1	37(1)
Br(2)	7332(1)	12902(1)	2153(1)	1	38(1)
Br(3)	8528(1)	10173(1)	1489(1)	1	36(1)
Br(4)	8207(1)	9927(1)	3699(1)	1	39(1)
Zn(1)	7560(1)	10626(1)	2257(1)	1	30(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{Bmpip})_2\text{ZnBr}_4$ at 293(2) K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br(1)	30(1)	38(1)	42(1)	-6(1)	12(1)	-2(1)
Br(2)	45(1)	29(1)	43(1)	-3(1)	20(1)	0(1)
Br(3)	30(1)	42(1)	36(1)	1(1)	14(1)	0(1)
Br(4)	43(1)	42(1)	31(1)	3(1)	12(1)	4(1)
Zn(1)	29(1)	30(1)	31(1)	-2(1)	11(1)	0(1)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$.

Table S3. Bond lengths [\AA] and Bond angles [$^\circ$] for $(\text{Bmpip})_2\text{ZnBr}_4$ at 293(2) K with estimated standard deviations in parentheses.

Label	Distances	Label	Angles
Br(1)-Zn(1)	2.4029(3)	Br(1)-Zn(1)-Br(2)	107.742(13)
Br(2)-Zn(1)	2.4199(3)	Br(1)-Zn(1)-Br(3)	108.451(13)
Br(3)-Zn(1)	2.4269(3)	Br(2)-Zn(1)-Br(3)	105.569(12)
Br(4)-Zn(1)	2.3991(3)	Br(4)-Zn(1)-Br(1)	112.141(13)
		Br(4)-Zn(1)-Br(2)	112.135(13)
		Br(4)-Zn(1)-Br(3)	110.513(13)

Symmetry transformations used to generate equivalent atoms:

(1) $-x, y + 1/2, -z + 1/2$ (2) $-x, -y, -z$ (3) $x, -y + 1/2, z + 1/2$.

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{Bmpip})_2\text{CdBr}_4$ at 293(2) K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Cd(1)	3877(1)	-392(1)	1240(1)	1	55(1)
Cd	8854(1)	-5101(1)	1244(1)	1	64(1)
Br(1)	9297(1)	-6791(2)	748(1)	1	73(1)
Br(4)	3907(5)	1060(6)	601(2)	0.522(2)	54(2)
Br(6B)	2879(4)	588(13)	1634(3)	0.64(7)	83(3)
Br(5)	5269(4)	-714(6)	1739(2)	0.522(2)	89(2)
Br(7B)	3222(15)	-2320(20)	901(7)	0.193(14)	201(9)
Br(B)	7743(2)	-6206(4)	1536(1)	0.851(8)	122(2)
Br(2)	9965(3)	-5099(4)	1907(2)	0.522(2)	100(2)
Br(3)	8684(3)	-2685(3)	919(2)	0.522(2)	100(2)
Br(A)	7428(7)	-5358(17)	1289(4)	0.149(8)	107(5)
Br(6A)	2908(11)	780(30)	1589(6)	0.36(7)	126(8)
Br(7A)	3556(3)	-2855(3)	1012(1)	0.807(14)	100(2)
Br(9)	9994(3)	-4395(4)	1848(2)	0.522(2)	97(2)
Br(10)	8314(4)	-3106(6)	800(2)	0.522(2)	154(2)
Br(11)	4072(6)	1204(10)	655(3)	0.478(2)	91(3)
Br(13)	5201(4)	-206(5)	1749(2)	0.478(2)	67(2)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{Bmpip})_2\text{CdBr}_4$ at 293(2) K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	55(1)	64(1)	46(1)	-12(1)	13(1)	2(1)
Cd	55(1)	90(1)	52(1)	-3(1)	20(1)	-13(1)
Br(1)	81(1)	77(1)	70(1)	-17(1)	38(1)	-18(1)
Br(4)	67(3)	60(2)	37(2)	-14(2)	16(2)	-2(2)
Br(6B)	69(3)	123(4)	69(3)	-1(3)	42(2)	9(3)
Br(5)	72(2)	143(5)	53(2)	35(3)	14(2)	7(3)
Br(7B)	178(14)	77(9)	280(20)	-57(9)	-96(16)	27(10)
Br(B)	103(2)	173(3)	115(2)	-54(2)	78(2)	-61(2)
Br(2)	119(3)	118(3)	51(2)	0(3)	-4(2)	17(2)
Br(3)	132(3)	67(2)	79(2)	27(2)	-25(2)	-11(2)
Br(9)	100(2)	125(3)	64(2)	-43(3)	17(2)	-26(2)
Br(10)	205(6)	146(4)	103(3)	93(4)	20(3)	-24(3)
Br(11)	62(3)	132(6)	85(4)	4(3)	29(3)	51(4)
Br(13)	55(2)	77(3)	60(2)	5(2)	-5(2)	-8(2)
Br(A)	92(8)	167(12)	76(7)	6(7)	44(6)	13(7)
Br(6A)	132(12)	175(11)	92(6)	64(11)	69(7)	74(11)
Br(7A)	128(2)	53(2)	108(2)	-25(2)	0(2)	5(1)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$.

Table S6. Bond lengths [\AA] for $(\text{Bmpip})_2\text{CdBr}_4$ at 293(2) K with estimated standard deviations in parentheses.

Label	Distances	Label	Distances
Cd(1)-Br(4)	2.574(7)	Cd-Br(1)	2.5870(13)
Cd(1)-Br(6B)	2.594(7)	Cd-Br(B)	2.603(2)
Cd(1)-Br(5)	2.647(7)	Cd-Br(2)	2.593(4)
Cd(1)-Br(7B)	2.384(12)	Cd-Br(3)	2.619(4)
Cd(1)-Br(11)	2.587(10)	Cd-Br(9)	2.591(4)
Cd(1)-Br(13)	2.555(6)	Cd-Br(10)	2.524(5)
Cd(1)-Br(6A)	2.539(18)	Cd-Br(A)	2.551(12)
Cd(1)-Br(7A)	2.585(2)		

Symmetry transformations used to generate equivalent atoms:

(1) $-x, y + 1/2, -z + 1/2$ (2) $-x, -y, -z$ (3) $x, -y + 1/2, z + 1/2$.

Table S7. Bond angles [$^\circ$] for $(\text{Bmpip})_2\text{CdBr}_4$ at 293(2) K with estimated standard deviations in parentheses.

Label	Angles	Label	Angles
Br(4)-Cd(1)-Br(5)	113.5(2)	Br(1)-Cd-Br(B)	108.52(6)
Br(4)-Cd(1)-Br(7A)	109.40(13)	Br(1)-Cd-Br(2)	105.36(13)
Br(7B)-Cd(1)-Br(6B)	103.3(7)	Br(1)-Cd-Br(3)	110.84(11)
Br(7B)-Cd(1)-Br(11)	105.6(6)	Br(1)-Cd-Br(9)	112.24(12)
Br(7B)-Cd(1)-Br(13)	129.9(8)	Br(2)-Cd-Br(3)	110.08(12)
Br(11)-Cd(1)-Br(6B)	111.3(4)	Br(9)-Cd-Br(B)	109.83(12)
Br(13)-Cd(1)-Br(6B)	104.8(2)	Br(10)-Cd-Br(1)	105.35(11)
Br(13)-Cd(1)-Br(11)	101.5(3)	Br(10)-Cd-Br(B)	109.5(2)
Br(6A)-Cd(1)-Br(4)	104.8(6)	Br(10)-Cd-Br(9)	111.32(19)
Br(6A)-Cd(1)-Br(5)	112.8(4)	Br(A)-Cd-Br(1)	114.1(3)
Br(6A)-Cd(1)-Br(7A)	116.2(6)	Br(A)-Cd-Br(2)	120.8(3)
Br(7A)-Cd(1)-Br(5)	100.34(17)	Br(A)-Cd-Br(3)	95.3(4)

Symmetry transformations used to generate equivalent atoms:

(1) $-x, y + 1/2, -z + 1/2$ (2) $-x, -y, -z$ (3) $x, -y + 1/2, z + 1/2$.

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{Bmpip})_8\text{Pb}_{11}\text{Br}_{30}$ at 293(2) K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Br	12325(11)	4231(19)	5004(3)	0.55(5)	47(3)
Br(2)	12516(10)	4565(14)	4974(4)	0.45(5)	34(2)
Br(3)	10626(2)	6427(1)	3610(1)	1	51(1)
Br(4)	9520(2)	4138(1)	3873(1)	1	44(1)
Br(5)	9860(1)	5994(1)	1767(1)	1	37(1)
Br(6)	6707(1)	5225(1)	2713(1)	1	44(1)
Br(7)	7713(2)	7626(1)	2606(1)	1	44(1)
Br(8)	7045(1)	6278(1)	125(1)	1	40(1)
Br(9)	8069(1)	8458(1)	325(1)	1	36(1)
Br(10)	7396(1)	8323(1)	-1705(1)	1	38(1)
Br(11)	4311(1)	7252(1)	-801(1)	1	37(1)
Br(12)	5116(1)	7515(1)	1586(1)	1	39(1)
Br(13)	7567(1)	10481(1)	1865(1)	1	42(1)
Br(14)	5365(1)	10371(1)	715(1)	1	32(1)
Br(15)	4452(2)	9368(1)	2849(1)	1	48(1)
Br(16)	5676(2)	11954(1)	3107(1)	1	56(1)
Pb(1)	10000	5000	5000	1	28(1)
Pb(2)	8628(1)	5817(1)	3318(1)	1	29(1)
Pb(3)	7492(1)	6716(1)	1501(1)	1	27(1)
Pb(4)	6051(1)	7921(1)	-228(1)	1	26(1)
Pb(5)	6345(1)	9048(1)	1691(1)	1	30(1)
Pb(6)	5234(1)	11205(1)	2059(1)	1	30(1)

* U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S9. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{Bmpip})_8\text{Pb}_{11}\text{Br}_{30}$ at 293(2) K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br	33(2)	66(8)	37(2)	15(4)	-5(2)	-15(2)
Br(2)	32(2)	40(5)	31(2)	4(3)	-4(2)	-15(2)
Br(3)	65(1)	43(1)	47(1)	-22(1)	-23(1)	0(1)
Br(4)	58(1)	28(1)	48(1)	2(1)	-14(1)	-10(1)
Br(5)	32(1)	49(1)	28(1)	-2(1)	-2(1)	-10(1)
Br(6)	35(1)	40(1)	50(1)	-11(1)	-12(1)	3(1)
Br(7)	60(1)	38(1)	48(1)	16(1)	-32(1)	-19(1)
Br(8)	53(1)	28(1)	48(1)	10(1)	-27(1)	-13(1)
Br(9)	31(1)	34(1)	40(1)	-6(1)	-6(1)	-6(1)
Br(10)	35(1)	44(1)	30(1)	4(1)	-2(1)	-10(1)
Br(11)	35(1)	31(1)	44(1)	-6(1)	-12(1)	-6(1)
Br(12)	31(1)	54(1)	29(1)	-8(1)	-6(1)	-4(1)
Br(13)	34(1)	50(1)	51(1)	2(1)	-17(1)	-20(1)
Br(14)	36(1)	33(1)	29(1)	5(1)	-14(1)	-10(1)
Br(15)	57(1)	38(1)	35(1)	0(1)	1(1)	2(1)
Br(16)	61(1)	73(1)	45(1)	0(1)	-13(1)	-36(1)
Pb(1)	29(1)	33(1)	23(1)	4(1)	-10(1)	-5(1)
Pb(2)	30(1)	33(1)	23(1)	4(1)	-10(1)	-5(1)
Pb(3)	31(1)	25(1)	26(1)	2(1)	-12(1)	-5(1)
Pb(4)	27(1)	27(1)	24(1)	3(1)	-9(1)	-4(1)
Pb(5)	36(1)	24(1)	33(1)	6(1)	-15(1)	-8(1)
Pb(6)	33(1)	29(1)	28(1)	1(1)	-9(1)	-8(1)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$.

Table S10. Bond lengths [Å] for $(\text{Bmpip})_8\text{Pb}_{11}\text{Br}_{30}$ at 293(2) K with estimated standard deviations in parentheses.

Label	Distances	Label	Distances
Br-Pb(1)	2.976(5)	Br(1)-Pb(4)	2.9894(11)
Br-Pb(2)#1	3.140(6)	Br(11)-Pb(6)#2	2.9853(11)
Br(2)-Pb(1)	3.036(8)	Br(12)-Pb(3)	3.0332(12)
Br(2)-Pb(2)#1	3.149(7)	Br(12)-Pb(5)	3.0870(12)
Br(3)-Pb(1)	3.0315(12)	Br(13)-Pb(5)	2.9953(12)
Br(3)-Pb(2)	2.8948(13)	Br(13)-Pb(6)	2.9316(12)
Br(4)-Pb(1)	3.0883(12)	Br(14)-Pb(4)#2	3.2283(11)
Br(4)-Pb(2)	2.9224(12)	Br(14)-Pb(5)	2.8806(11)
Br(5)-Pb(2)	2.9370(12)	Br(14)-Pb(6)	3.2216(11)
Br(5)-Pb(3)	3.1080(12)	Br(15)-Pb(5)	2.8821(13)
Br(6)-Pb(2)	3.1492(12)	Br(15)-Pb(6)	3.0932(12)
Br(6)-Pb(3)	2.9250(12)	Br(16)-Pb(6)	2.8130(13)
Br(7)-Pb(2)	3.1811(12)	Pb(1)-Br#1	2.976(5)
Br(7)-Pb(3)	2.9917(12)	Pb(1)-Br(2)#1	3.036(8)
Br(7)-Pb(5)	3.1717(11)	Pb(1)-Br(3)#1	3.0315(12)
Br(8)-Pb(3)	3.1217(12)	Pb(1)-Br(4)#1	3.0883(12)
Br(8)-Pb(4)	2.8629(11)	Pb(2)-Br#1	3.140(6)
Br(9)-Pb(3)	3.1445(11)	Pb(2)-Br(2)#1	3.149(7)
Br(9)-Pb(4)	3.1460(11)	Pb(4)-Br(14)#2	3.2282(11)
Br(10)-Pb(4)	2.8279(12)	Pb(6)-Br(11)#2	2.9853(12)

Symmetry transformations used to generate equivalent atoms:

(1) $-x + 2, -y + 1, -z + 1$ (2) $-x + 1, -y + 2, -z$.

Table S11. Bond angles [°] for (Bmpip)₈Pb₁₁Br₃₀ at 293(2) K with estimated standard deviations in parentheses.

Label	Angles	Label	Angles
Pb(1)-Br-Pb(2)	79.30(13)	Br(3)-Pb(2)-Br(7)	95.69(4)
Pb(1)-Br(2)-Pb(2)	78.3(2)	Br(4)-Pb(2)-Br	84.6(4)
Pb(2)-Br(3)-Pb(1)	82.40(3)	Br(4)-Pb(2)-Br(2)	77.7(3)
Pb(2)-Br(4)-Pb(1)	80.98(3)	Br(4)-Pb(2)-Br(5)	95.67(4)
Pb(2)-Br(5)-Pb(3)	82.35(3)	Br(4)-Pb(2)-Br(6)	96.36(3)
Pb(3)-Br(6)-Pb(2)	81.83(3)	Br(4)-Pb(2)-Br(7)	176.13(4)
Pb(3)-Br(7)-Pb(2)	80.27(3)	Br(5)-Pb(2)-Br	170.5(5)
Pb(3)-Br(7)-Pb(5)	82.53(3)	Br(5)-Pb(2)-Br(2)	173.2(2)
Pb(5)-Br(7)-Pb(2)	160.66(4)	Br(5)-Pb(2)-Br(6)	79.20(3)
Pb(4)-Br(8)-Pb(3)	87.35(3)	Br(5)-Pb(2)-Br(7)	80.60(3)
Pb(3)-Br(9)-Pb(4)	82.25(3)	Br(6)-Pb(2)-Br(7)	81.95(3)
Pb(6)-Br(11)-Pb(4)	86.65(3)	Br(5)-Pb(3)-Br(8)	110.47(3)
Pb(3)-Br(12)-Pb(5)	83.29(3)	Br(5)-Pb(3)-Br(9)	105.28(3)
Pb(6)-Br(13)-Pb(5)	81.96(3)	Br(6)-Pb(3)-Br(5)	80.06(3)
Pb(5)-Br(14)-Pb(4)	156.99(4)	Br(6)-Pb(3)-Br(7)	89.09(4)
Pb(5)-Br(14)-Pb(6)	78.93(3)	Br(6)-Pb(3)-Br(8)	104.20(4)
Pb(6)-Br(14)-Pb(4)	78.93(3)	Br(6)-Pb(3)-Br(9)	171.99(4)
Pb(5)-Br(15)-Pb(6)	81.08(3)	Br(7)-Pb(3)-Br(5)	80.98(3)
Br-Pb(1)-Br	180.000(3)	Br(7)-Pb(3)-Br(8)	163.57(3)
Br-Pb(1)-Br(2)	168.7(2)	Br(7)-Pb(3)-Br(9)	85.92(3)
Br-Pb(1)-Br(2)	168.7(2)	Br(7)-Pb(3)-Br(12)	86.43(3)
Br-Pb(1)-Br(2)	11.3(2)	Br(8)-Pb(3)-Br(9)	79.75(3)
Br-Pb(1)-Br(2)	11.3(2)	Br(12)-Pb(3)-Br(5)	166.61(3)
Br-Pb(1)-Br(3)	99.8(4)	Br(12)-Pb(3)-Br(8)	82.81(3)
Br-Pb(1)-Br(3)	80.2(4)	Br(12)-Pb(3)-Br(9)	78.18(3)
Br-Pb(1)-Br(3)	80.2(4)	Br(8)-Pb(4)-Br(9)	83.78(3)
Br-Pb(1)-Br(3)	99.8(4)	Br(8)-Pb(4)-Br(11)	90.39(3)
Br-Pb(1)-Br(4)	95.4(5)	Br(8)-Pb(4)-Br(14)	170.70(3)
Br-Pb(1)-Br(4)	84.6(5)	Br(9)-Pb(4)-Br(14)	105.52(3)
Br-Pb(1)-Br(4)	95.4(5)	Br(10)-Pb(4)-Br(8)	93.48(4)
Br-Pb(1)-Br(4)	84.6(5)	Br(10)-Pb(4)-Br(9)	91.35(3)
Br(2)-Pb(1)-Br(2)	180.000(1)	Br(10)-Pb(4)-Br(11)	85.95(3)
Br(2)-Pb(1)-Br(4)	103.0(3)	Br(10)-Pb(4)-Br(14)	86.15(3)
Br(2)-Pb(1)-Br(4)	77.0(3)	Br(11)-Pb(4)-Br(9)	173.42(3)
Br(2)-Pb(1)-Br(4)	77.0(3)	Br(11)-Pb(4)-Br(14)	80.31(3)
Br(2)-Pb(1)-Br(4)	103.0(3)	Br(12)-Pb(5)-Br(7)	82.46(3)
Br(3)-Pb(1)-Br(2)	87.2(3)	Br(13)-Pb(5)-Br(7)	94.85(3)
Br(3)-Pb(1)-Br(2)	87.2(3)	Br(13)-Pb(5)-Br(12)	177.04(3)
Br(3)-Pb(1)-Br(2)	92.8(3)	Br(14)-Pb(5)-Br(7)	172.83(4)

Br(3)-Pb(1)-Br(2)	92.8(3)	Br(14)-Pb(5)-Br(12)	99.55(3)
Br(3)-Pb(1)-Br(3)	180.0	Br(14)-Pb(5)-Br(13)	83.28(3)
Br(3)-Pb(1)-Br(4)	80.25(3)	Br(14)-Pb(5)-Br(15)	85.64(3)
Br(3)-Pb(1)-Br(4)	80.25(3)	Br(15)-Pb(5)-Br(7)	101.19(4)
Br(3)-Pb(1)-Br(4)	99.75(3)	Br(15)-Pb(5)-Br(12)	92.48(4)
Br(3)-Pb(1)-Br(4)	99.75(3)	Br(15)-Pb(5)-Br(13)	86.82(4)
Br(4)-Pb(1)-Br(4)	180.0	Br(11)-Pb(6)-Br(14)	80.48(3)
Br-Pb(2)-Br(2)	10.83(18)	Br(11)-Pb(6)-Br(15)	155.67(4)
Br-Pb(2)-Br(6)	110.3(4)	Br(13)-Pb(6)-Br(11)	99.41(3)
Br-Pb(2)-Br(7)	99.3(4)	Br(13)-Pb(6)-Br(14)	78.63(3)
Br(2)-Pb(2)-Br(6)	102.5(3)	Br(13)-Pb(6)-Br(15)	84.17(4)
Br(2)-Pb(2)-Br(7)	106.1(3)	Br(15)-Pb(6)-Br(14)	76.64(3)
Br(3)-Pb(2)-Br	79.7(4)	Br(16)-Pb(6)-Br(11)	95.95(4)
Br(3)-Pb(2)-Br(2)	87.5(3)	Br(16)-Pb(6)-Br(13)	89.51(4)
Br(3)-Pb(2)-Br(4)	85.38(4)	Br(16)-Pb(6)-Br(14)	166.80(4)
Br(3)-Pb(2)-Br(5)	90.84(4)	Br(16)-Pb(6)-Br(15)	108.18(4)
Br(3)-Pb(2)-Br(6)	170.01(4)		

Symmetry transformations used to generate equivalent atoms:

(1) $-x + 2, -y + 1, -z + 1$ (2) $-x + 1, -y + 2, -z$.

Table S12. Bond length and bond angle average and distortion of individual $[\text{PbBr}_6]$ octahedra of $(\text{Bmpip})_8\text{Pb}_{11}\text{Br}_{30}$ (θ_m is the mean value of Br-Pb-Br angles).

Label	Pb1	Pb2	Pb3	Pb4	Pb5	Pb6	Average
d_m (Å)	3.042	3.038	3.054	3.060	3.072	3.043	3.0515
θ_m (°)	90.000	89.955	89.870	90.150	89.313	90.076	89.894
$\Delta d (\times 10^{-4})$	1.3	16.0	6.5	34.3	38.1	20.3	19.4
σ^2	80.0	86.0	126.3	105.0	163.0	79.8	106.7

Table S13. Main parameters of crystal and refinement power of $(\text{Bmpip})_2\text{ZnBr}_4$.

Status	Crystal	Power
a (Å)	16.3329	16.5138
b (Å)	10.5189	10.7468
c (Å)	16.9147	16.9680
β (°)	111.10	110.102
V (Å ³)	2711.1	2827.87
R_p (%)		13.6
R_{wp} (%)		15.7
R_{exp} (%)		7.86
χ^2		3.98

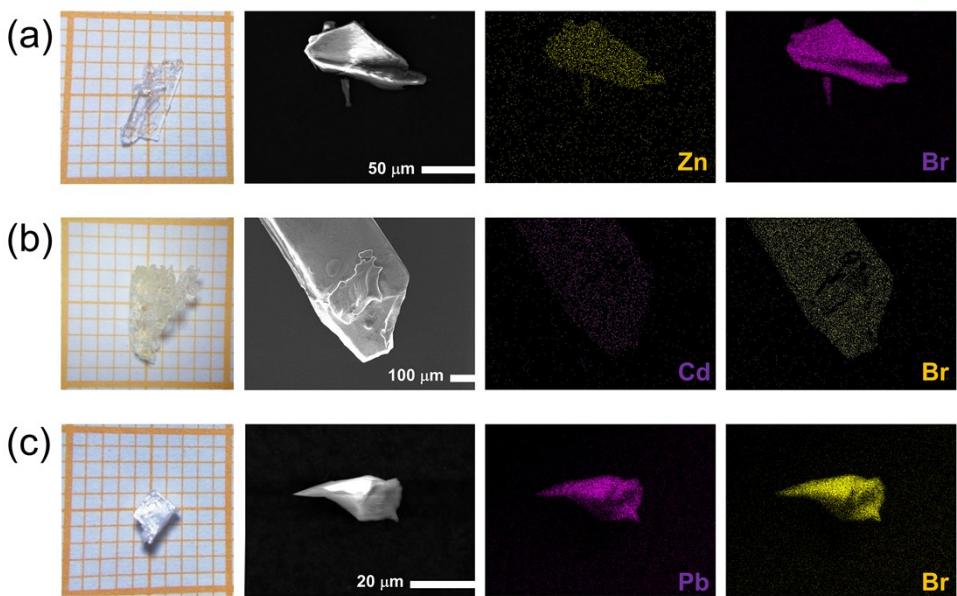


Fig. S1 Optical and SEM images and EDS mapping diagrams of $(\text{Bmpip})_2\text{ZnBr}_4$ (a), $(\text{Bmpip})_2\text{CdBr}_4$ (b) and $(\text{Bmpip})_8\text{Pb}_{11}\text{Br}_{30}$ (c).

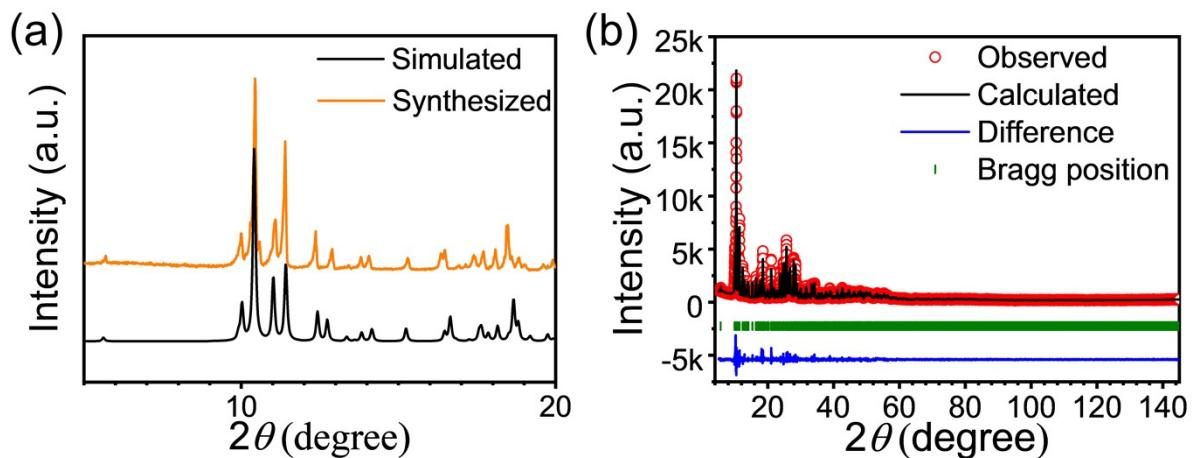


Fig. S2 (a) Local details of simulated and experimental PXRD patterns. (b) Rietveld refinement of $(\text{Bmpip})_2\text{ZnBr}_4$.

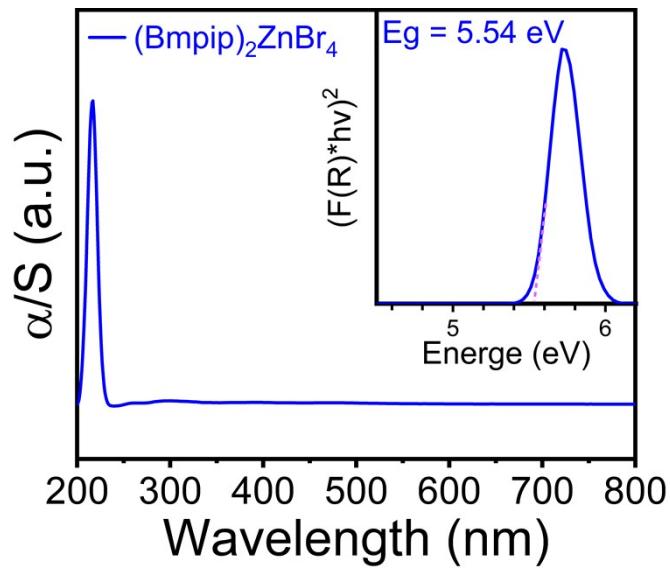


Fig. S3 Absorption spectra and the band gap obtained from Tauc plots (inset) of $(\text{Bmpip})_2\text{ZnBr}_4$.

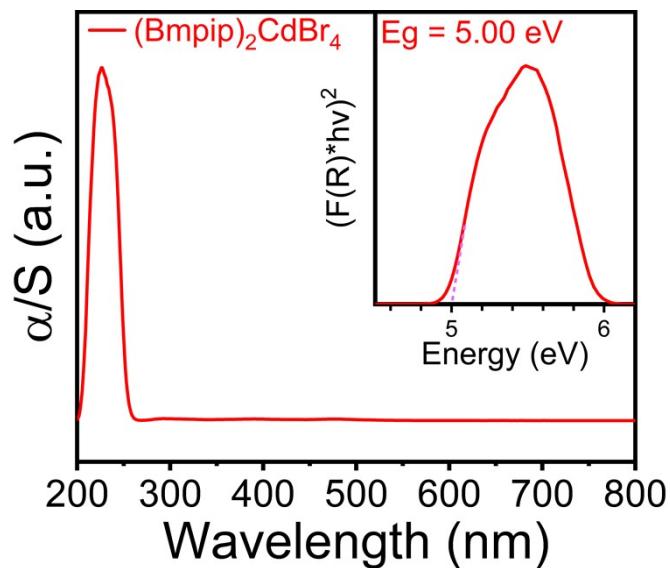


Fig. S4 Absorption spectra and the band gap obtained from Tauc plots (inset) of $(\text{Bmpip})_2\text{CdBr}_4$.

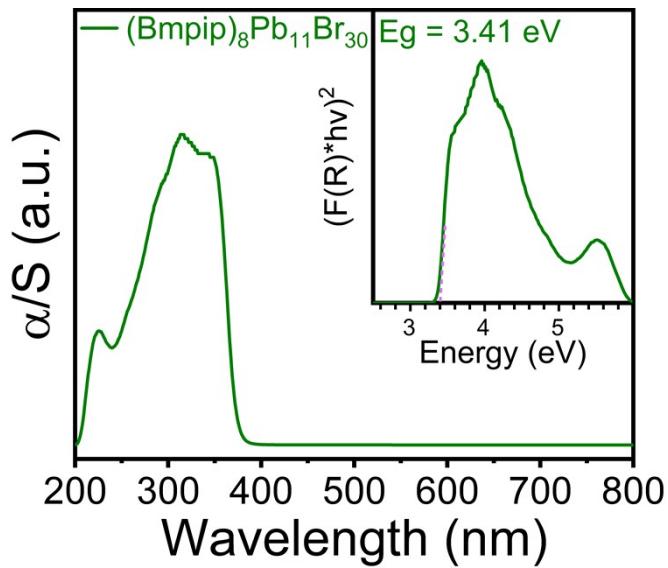


Fig. S5 Absorption spectra and the band gap obtained from Tauc plots (inset) of $(\text{Bmpip})_8\text{Pb}_{11}\text{Br}_{30}$.

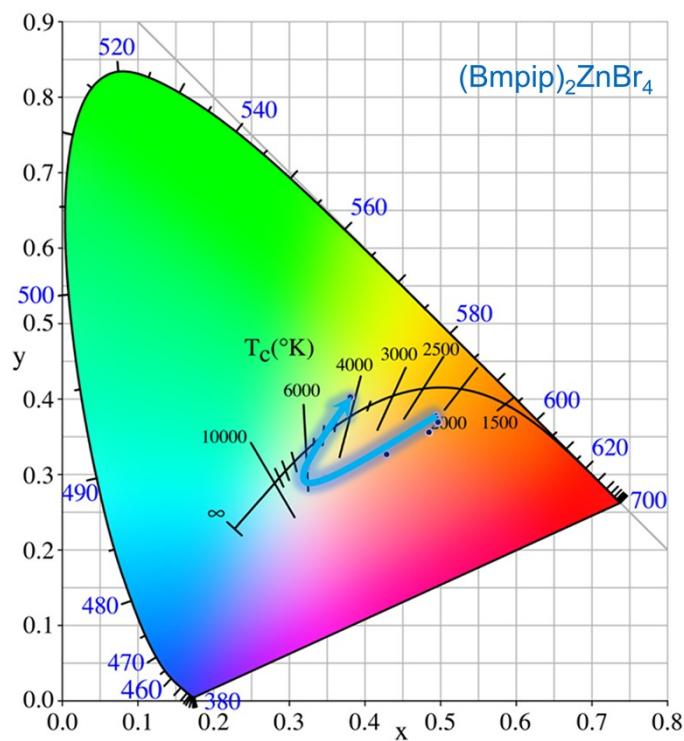


Fig. S6 CIE coordinates change with temperature increasing of $(\text{Bmpip})_2\text{ZnBr}_4$.

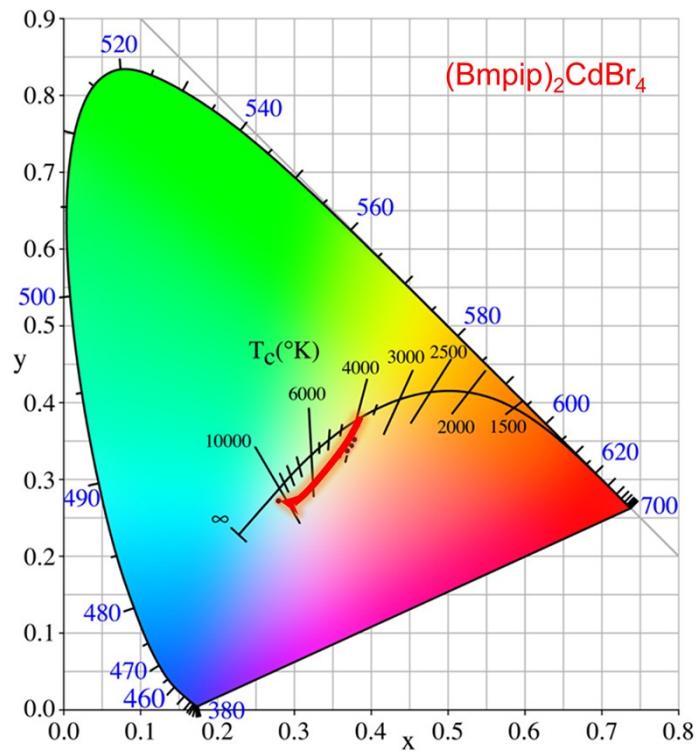


Fig. S7 CIE coordinates change with temperature increasing of $(\text{Bmpip})_2\text{CdBr}_4$.

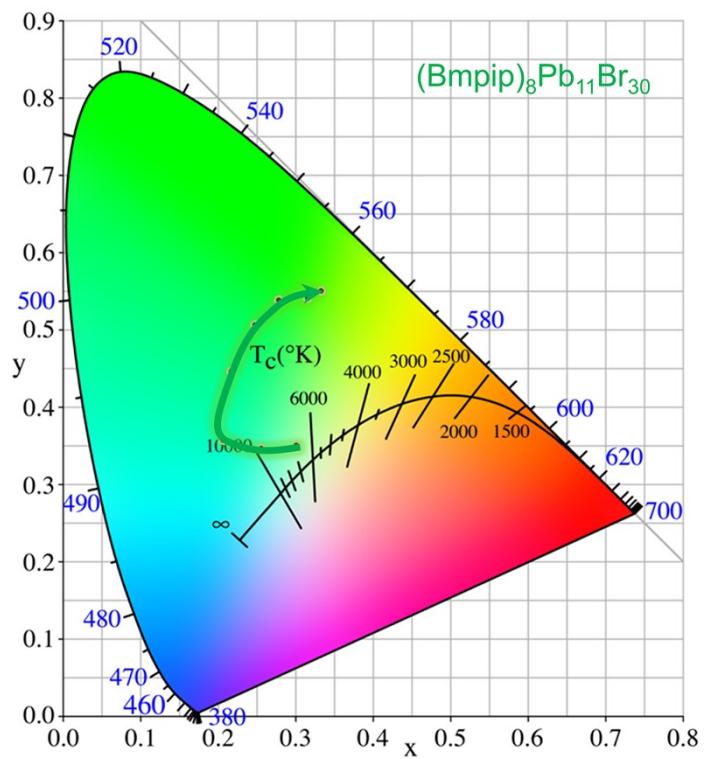


Fig. S8 CIE coordinates change with temperature increasing of $(\text{Bmpip})_8\text{Pb}_{11}\text{Br}_{30}$.